

Idoxuridine

54-42-2 | DTXSID2045238

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.14×10^{-11} cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.79×10^{-1}

Confidence level: 8.31×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Bornyl acetate

Measured: 1.39×10^{-11}

Predicted: 1.36×10^{-11}

Image not found

Dimethyl adipate

Measured: 8.40×10^{-12}

Predicted: 6.84×10^{-12}

Image not found

Isoproturon

Measured: 1.20×10^{-11}

Predicted: 3.23×10^{-11}

Image not found

Dimethyl glutarate

Measured: 3.30×10^{-12}

Predicted: 3.76×10^{-12}